4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

The common synonyms and other information for fluorine, hydrogen fluoride, and sodium fluoride are listed in Table 4-1. The terms "fluorine" and "fluoride" are often used interchangeably in the literature as generic terms. In this document, we will use the terms "fluoride" as a general term to refer to all combined forms of fluorine unless the particular compound or form is known and there is a reason for referring to it. We will sometimes use the term "fluorine gas" to emphasize the fact that we are referring to the elemental form of fluorine rather than a combined form. In general, the differentiation between different ionic and molecular or gaseous and particulate forms of fluorine-containing substances is uncertain and may also be unnecessary.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Fluorine is the lightest member of Group 17 (VIIA) of the periodic table. This group, the halogens, also includes chloride, bromine, and iodine. As with the other halogens, fluorine occurs as a diatomic molecule, F_2, in its elemental form. It has only one stable isotope and its valence in all compounds is -1. Fluorine is the most reactive of all the elements, which may be attributed to its large electronegativity (estimated standard potential +2.85 V). It reacts at room temperature or elevated temperatures with all elements other than nitrogen, oxygen, and the lighter noble gases. Fluorine is also notable for its small size; large numbers of fluorine atoms fit around atoms of another element. This, along with its electronegativity, allows the formation of many simple and complex fluorides in which the other element is in its highest oxidation date. Important physical and chemical properties of fluorine, hydrogen fluoride, and sodium fluoride are presented in Table 4-2.

Table 4-1. Chemical Identity of Fluorine, Hydrogen Fluoride, and Sodium Fluoride[a]

Characteristic	Fluorine	Hydrogen fluoride	Sodium fluoride
Synonym(s)	Fluorine-19	Hydrofluoric acid; hydrofluoride	Monosodium fluroride[b]
Registered trade name(s)	No data	No data	Alcoa sodium fluoride[b]
Chemical formula	F_2	FH	FNa
Chemical structure	F-F	H-F	Na-F
Identification numbers:			
CAS registry	7782-41-4	7664-39-3	7681-49-4
NIOSH RTECS	NIOSH/LM64750000	NIOSH/MW7890000	NIOSH/WB0350000
EPA hazardous waste	P056	U134	No data
OHM/TADS	No data	7216750	7216897
DOT/UN/NA/IMO shipping	UN1045; fluorine	UN1790; hydrofluoric acid solution UN1052; anhydrous hydrogen fluoride	UN1690; sodium fluoride
HSDB	541	546	1766
EINECS	231-954-8	231-634-8	231-667-8
NCI	No data	No data	C55221

[a]All information obtained from HSDB 2001 and ChemID 2001 except where noted.
[b]Sodium fluoride is an ingredient in many dental care products and rodenticides. Since it is not the only component in these products, they cannot properly be considered trade names or synonyms. Some of these products are: Floridine, Antibulit, Cavi-trol, Chemifluor, Credo, Duraphat, F1-tabs, Florocid, Flozenges, Fluoral, Fluorident, Fluorigard, Fluorineed, Fluorinse, Fluoritab, Fluorocid, Fluor-o-kote, Fluorol, Fluoros, Flura, Flura drops, Flura-gel, Flura-Loz, Flurcare, Flursol, Fungol B, Gel II, Gelution, Gleem, Iradicav, Karidium, Karigel, Kari-rinse, Lea-Cov, Lemoflur, Luride, Luride Lozi-tabs, Luride-SF, Nafeen, Nafpak, Na Frinse, Nufluor, Ossalin, Ossin, Osteofluor, Pediaflor, Pedident, Pennwhite, Pergantene, Phos-flur, Point Two, Predent, Rafluor, Rescue Squad, Roach salt, So-flo, Stay-flo, Studafluor, Super-dent, T-fluoride, Thera-flur, Thera-Flur-N, Villiaumite, Zymafluor. Another compound of sodium and fluorine is sodium bifluoride (also called sodium hydrofluoride and sodium hydrofluoride), $NaF·HF$ or $NaHF_2$, which is not discussed here.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Oganization Code; EINECS = European INventory of Existing Chemical Substances; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/ Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Physical and Chemical Properties of Fluorine, Hydrogen Fluoride, and Sodium Fluoride[a]

Property	Fluorine	Hydrogen fluoride	Sodium fluoride
Molecular weight	37.997	20.006	42.00
Color	Pale yellow	Colorless	Colorless
Physical state	Gas	Gas	Cubic or tetragonal crystals
Molecular formula	F_2	FH	FNa
Melting point, EC	-219.61	-83.36	993
Boiling point, EC	-188.13	19.51[b]	1,704
Density, g/cm^3	1.5127 at -188.13 EC	0.991 at 19.54 EC	2.78
Odor	Pungent, irritating odor	Strong, irritating odor	Odorless
Odor threshold:			
Water	Not relevant	No data	No data
Air	0.035 ppm	0.5–3 ppm	No data
Solubility:			
Water	1.69 mg/L	Miscible	43 g/L at 25 EC
Organic solvents, weight. % at 5 EC	No data	Benzene (2.54); toluene (1.80); ethanol (very soluble); *m*-xylene (1.28); tetraline (0.27)[b]	Very slightly soluble in ethanol
Partition coefficients:			
Log K_{ow}	Not relevant	No data	No data
Log K_{oc}	Not relevant	Not relevant	No data
Vapor pressure	0.4 kPa (3 mmHg) at 55 K[c] 12.3 kPa (92.3 mmHg) at 70 K	400 mmHg at 2.5 EC	1 mmHg at 1,077 EC
Henry's law constant at 20 EC	No data	0.104 atm-L/mole[e]	No data

Table 4-2. Physical and Chemical Properties of Fluorine, Hydrogen Fluoride, and Sodium Fluoride[a] *(continued)*

Property	Fluorine	Hydrogen fluoride	Sodium fluoride
Autoignition temperature	No data	No data	No data
Flashpoint	Not flammable	Not flammable	Not flammable
Flammability limits	No data	No data	No data
Conversion factors	1 mg/m^3 = 1.554 ppm[d] 1 ppm = 0.64 mg/m^3	1 mg/m^3 = 1.223 ppm[d] 1 ppm = 0.82 mg/m^3	Not applicable
Explosive limits	No data	No data	No data

[a]All information obtained from HSDB 2001 except where noted
[b]Budavari 1996
[c]Lide 1992
[d]NAS 1971a
[e]Betterton 1992; apparent Henry's law constant (ratio of the gas phase concentration to that of the total dissolved solute)